RGC Ref.: N_HKUST 603/15 NSFC Ref. : 21561162001
(please insert ref. above)

The Research Grants Council of Hong Kong
NSFC/RGC Joint Research Scheme
Joint Completion Report

(Please attach a copy of the completion report submitted to the NSFC by the Mainland researcher)

Part A: The Project and Investigator(s)

1. Project Title

Design, synthesis and application of fused osmacycles/iridacycles containing main group heteroatoms

2. Investigator(s) and Academic Department/Units Involved

	Hong Kong Team	Mainland Team
Name of Principal Investigator *(with title)*	Zhenyang Lin (Chair Professor)	Haiping Xia (Professor)
Post	Chair Professor	Professor
Unit / Department / Institution	Department of Chemistry HKUST	Department of Chemistry Xiamen University
Contact Information	chzlin@ust.hk	hpxia@xmu.edu.cn
Co-investigator(s) *(with title and institution)*		Professor Hong Zhang Xiamen University

3. Project Duration

	Original	Revised	Date of RGC/ Institution Approval *(must be quoted)*
Project Start date	1 January 2016		
Project Completion date	31 December 2019		
Duration *(in month)*	48 months		
Deadline for Submission of Completion Report	31 December 2020		

Part B: The Completion Report

5. Project Objectives

5.1 Objectives as per original application

1. To construct fused osmacycles/iridacycles by calculating/comparing feasible reaction pathways derived from various starting materials through DFT calculations and experiments.
2. To examine factors influencing the stability, reactivity and properties of various fused osmacycles/iridacycles by studying their electronic structures.
3. To examine whether and how a main group heteroatom in a given metallacycle affects the reactivity and properties of osmacycles/iridacycles.

5.2 Revised Objectives (Not Applicable)

Date of approval from the RGC: _____

Reasons for the change: _____

_____

1.
2.
3. ....

6. Research Outcome

Major findings and research outcome
(maximum 1 page; please make reference to Part C where necessary)

A number of new osmacycle/iridacycle complexes have been synthesized (See Entries 1, 6, 7 and 8 in Section 8).

The newly synthesized complexes display interesting reactivities (electrophilic and nucleophilic) and physical properties (luminescent) that allow for further studies (See Entries 1, 2, 4, 7 and 8 in Section 8).

Interesting electronic structures and bonding that impact reactivity and physical properties were examined and identified in the newly synthesized complexes (Entries 3, 5 and 9 in Section 8).

Potential for further development of the research and the proposed course of action
(maximum half a page)

Systematic way on the synthesis of metallocycle complexes can be developed when more studies in the related area are completed.

Systematic understanding of the physical properties needs to be developed, and application of the newly synthesized metallocycle complexes requires further studies.

7. The Layman's Summary

(describe <u>in layman's language</u> the nature, significance and value of the research project, in no more than 200 words)

In this completed projects, a series of new metallacyclic organometallic compounds have been prepared and characterized. Investigation of their physical properties indicate that these compounds display potential photoluminescence that deserves for further studies. Synthetic investigation also allows us to modify the structures and incorporation of hetero atoms into the metallacycle rings and studies of the effect of the heteroatom on their chemical and physical properties.

<u>Part C: Research Output</u>

8. Peer-reviewed journal publication(s) arising <u>directly</u> from this research project

(Please attach a copy of each publication and/or the letter of acceptance if not yet submitted in the previous progress report(s). All listed publications must acknowledge RGC's funding support by quoting the specific grant reference.)

The Latest Status of Publications				Author(s) ***(bold** the authors belonging to the project teams and denote the corresponding author with an asterisk*)*	Title and Journal/ Book *(with the volume, pages and other necessary publishing details specified)*	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
Year of publication	Year of Acceptance *(For paper accepted but not yet published)*	Under Review	Under Preparation *(optional)*						
2017 (Entry 1) J1				Ming Luo, Lipeng Long, Hong Zhang,* Yuhui Yang, Yuhui Hua, Gang Liu, Zhenyang Lin,* and Haiping Xia*	"Reactions of Isocyanides with Metal Carbyne Complex: Isolation and Characterization of Metallacyclopropenimine Intermediates" *J. Amer. Chem. Soc*., **139**, 1822-1825.	Dec 2017	No (submitted in the previous progress report)	Yes	Yes
2017 (Entry 2) J2				Zi-Ao Huang, Qing Lan, Yuhui Hua, Zhixin Chen, Hong Zhang,* Zhenyang Lin and Haiping Xia	"Color-tuning strategy for iridapolycycles $[(N^N)Ir(C^C)ClPPh_3]^+$ by the synergistic modifications on both the C^C and N^N units" *Organometallics*, **36**, 4802-4809.	Dec 2017	No (submitted in the previous progress report)	Yes	Yes
2017 (Entry 3) J3				Fu Kit Sheong, Jing-Xuan Zhang and Zhenyang Lin*	"Localized Bonding Model for Coordination and Cluster Compounds" *Coord. Chem. Rev*. **345**, 42-53.	Dec 2017	No (submitted in the previous progress report)	Yes	Yes
2017 (Entry 4) J4				Hao Wang, Linlin Wu, Zhenyang Lin* and Zuowei Xie*	"Synthesis, Structure and Reactivity of a Borylene Cation $[(NHSi)_2B(CO)]^+$ Stabilized by Three Neutral Ligands" *J. Amer. Chem. Soc*., **139**, 13680-13683.	Dec 2017	No (submitted in the previous progress report)	Yes	Yes

2018 (Entry 5) J5				Jing-Xuan Zhang, Fu Kit Sheong* and Zhenyang Lin*	"Unravelling Chemical Interactions with Principal Interacting Orbitals" *Chemistry - A European Journal*, **24**, 9639-9650	Nov 2020	Yes	Yes	Yes
2019 (Entry 6) J6				Jinhua Li, Yu-Mei Lin,* Hong Zhang, Yuan Chen, Zhenyang Lin, and Haiping Xia*	"Access to Metal-bridged Osmathiazine Derivatives by a Formal [4+2] Cyclization" *Chemistry - A European Journal*, **25**, 5077-5085	Nov 2020	Yes	Yes	Yes
2019 (Entry 7) J7				Xiaoxi Zhou, Xin Pang, Liming Nie, Congqing Zhu, Kaiyue Zhuo, Qingde Zhuo, Zhixin Chen, Gang Liu, Hong Zhang,* Zhenyang Lin and Haiping Xia	"Successive modification of polydentate complexes gives access to planar carbon- and nitrogen-based ligands" *Nature Communications*, **10**, 1488	Nov 2020	Yes	Yes	Yes
2020 (Entry 8) J8				Ming Luo, Yuhui Hua, Kaiyue Zhuo, Lipeng Long, Xinlei Lin, Zhihong Deng, Zhenyang Lin, Hong Zhang, Dafa Chen, and Haiping Xia*	"Carbolong Chemistry: Planar CCCCX-type (X = N, O, S) Pentadentate Chelates by Formal [3+1] Cycloadditions of Metalla-Azirines with Terminal Alkynes" *CCS Chemistry*, **2**, 758-763	Nov 2020	Yes	Yes	Yes
2020 (Entry 9) J9				Jing-Xuan Zhang, Fu Kit Sheong (co-first author), Zhengyu Lu, Hong Zhang* and Zhenyang Lin*	"Unexpected electronic behavior of organic azide and metal-carbyne in their 1,3-dipolar cycloaddition reaction" *Chinese J. Chem.*, **38**, 1565-1570	Nov 2020	Yes	Yes	Yes

9. Recognized international conference(s) in which paper(s) related to this research project was/were delivered *(Please attach a copy of each delivered paper. All listed papers must acknowledge RGC's funding support by quoting the specific grant reference.)*

	Month/Year/ Place	Title	Conference Name	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
C1	June/2017/ Xiamen	Transition Metal Boryl Complexes and Catalysis – Insights form Computational Studies	New Frontiers in Organometallic Chemistry	December 2017	No (submitted in the previous progress report)	Yes	No
C2	Nov/2018/ Wuhan	Transition Metal Catalyzed Reactions of Carbon Dioxide - Computational Insight	Wuhan Conference on Green Chemistry and Sustainable Catalysis 2018	Nov 2020	Yes	Yes	Yes
C3	Feb/2019/ Bangkok, Thailand	Unravelling chemical interactions with Principal Interacting Orbital (PIO) analysis	Pure and Applied Chemistry International Conference – PACCON 2019	Nov 2020	Yes	Yes	Yes
C4	Sept/2019/ Stockholm, Sweden	Boryls, Their Metal Complexes and Catalysis - Theoretical and Computational Insights	Mechanistic Homogeneous Catalysis - A Meeting between Theory and Experiment	Nov 2020	Yes	Yes	Yes

10. Student(s) trained *(Please attach a copy of the title page of the thesis.)*

	Name	Degree registered for	Date of registration	Date of thesis submission/ graduation
S1	Zheng WANG	PhD	1 September 2013	31 August 2017
S2	Linlin WU	PhD	1 September 2014	31 August 2018
S3	Jingxuan ZHANG	PhD	1 September 2014	31 August 2018

11. Other impact *(e.g. award of patents or prizes, collaboration with other research institutions, technology transfer, etc.)*

Close collaboration between my research group in Hong Kong and Prof Haiping Xia's research group in Xiamen has been well established in the area of metallocyclic organometallic chemistry.

12. Statistics on Research Outputs *(Please ensure the summary statistics below are consistent with the information presented in other parts of this report.)*

	Peer-reviewed journal publications	Conference papers	Scholarly books, monographs and chapters	Patents awarded	Other research outputs (Please specify)
No. of outputs arising directly from this research project [or conference]	9	4	N.A.	N.A.	N.A.